

rotation_zhulab

Record work every week and save in . /Progress

Dec_28_2019

MSA-based approach development

Selecting the appropriate mutation site based on the information of protein evolution

- mutiple sequence alignment
- distance map --> hydrogen bond ditinguish
- 3D visualization

MSA-independent approach exploration

information beyond protein evolution: mutation?

see detail in

This browser does not support PDFs. Please download the

PDF to view it: [Download PDF](#).

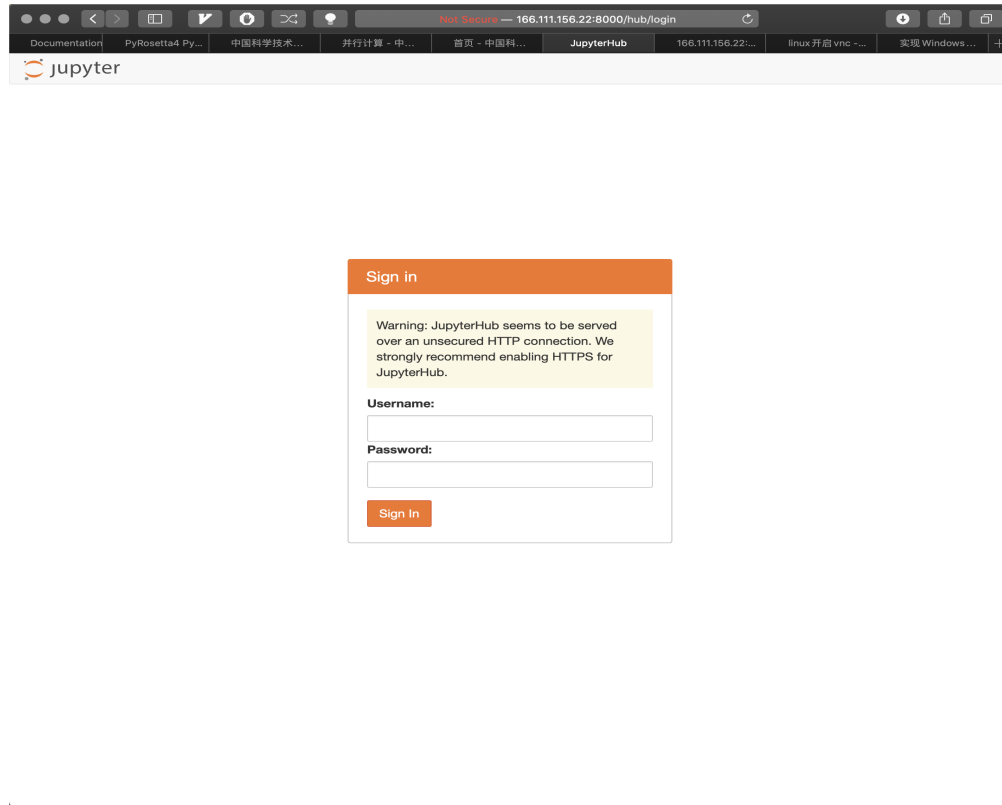
server&cluster env

cluster

install rosetta on cluster, pyrosetta failed because of error GLIBC.2.17 not found , contact Anbao and solve the problem

server

install `jupyterhub` and we can type `http://166.111.156.22:8000` on browsers and sign in our server. Do visualization work as we can: like `matplotlib` plotting



peer

Yunxin Xu in Haipeng Gong lab does similar work: de novo protein folding by `pyrosetta` and `trRosetta`, chat with him to promote my work

Jan_06_2019

aim: mutate, Ile, split(know what is split, previous method about split in `reading_list`)

paper reading about split

MSA-based approach

- mutiple sequence alignment (experienced but to do)
- distance map --> hydrogen bond ditinguish (to do, not too hard)
- 3D visualization (doing)

server (166.111.156.22)

teamviewer (desktop remote) linux service

`pymol`

so we can open PDB file on server and have a vision of protein 3D structure

trRosetta

from sequence file to PDB file

```
python trRosetta.py T1008.npz T1008.fasta model.pdb
```

T1008.npz is like distance map, can also derive from fasta
so we can have 3D visualization of mutant protein.

website (zhulab)

| software | function |
|----------|--|
| nginx | can browse IP:port to get data in computer (modify nginx.conf) |
| Vscode | install live server plugin to see website in-time and modify html file and see direct effect |

update new html file to the website-server

learning

Data structure

Parallel Computing